

# Evolution of the CPT Invariance into a Basic Postulate in Physics

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Einstein-Podolsky-Rosen's paper in 1935 is discussed in parallel with an EPR experiment on  $K^0\bar{K}^0$  system in 1998, yielding a strong hint of distinction in both wave-function and operators between particle and antiparticle at the level of quantum mechanics (QM). Then it is proposed that the CPT invariance in particle physics leads naturally to a basic postulate that the (newly defined) space-time inversion ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) is equivalent to the transformation between particle and its antiparticle. The evolution of this postulate from nonrelativistic QM via relativistic QM till the quantum field theory is discussed in some detail. The Klein paradox for both Klein-Gordon equation and Dirac equation is also discussed.

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## I. INTRODUCTION

The famous paper by Einstein, Podolsky and Rosen (EPR [1]) in 1935 is not easy to read, at least to us. And the deep implication of a remarkable experiment performed by the CPLEAR collaboration in 1998 [2] is not easy to explore either. In this paper we will discuss them in parallel in section II before we will be able to extract some new conception

via their combination. Then in section III, a new postulate emerged from the research on the CPT invariance in particle physics will be proposed. The evolution of its form from quantum mechanics (QM) via relativistic QM (RQM) till quantum field theory (QFT) will be discussed in section IV. The final section V will be a brief summary and discussion. The Klein paradox for both Klein-Gordon (KG) equation and Dirac equation is discussed in an Appendix.

## II. WHAT THE $K^0\bar{K}^0$ CORRELATION EXPERIMENTAL DATA ARE TELLING?

To our knowledge, beginning from Bohm [3] and Bell [4], physicists gradually turned their research of EPR paradox onto the entangled state composed of electrons, especially photons with spin and achieved fruitful results. However, as pointed out by Guan (1935-2007), EPR's paper [1] is focused on two spinless particles and Guan found that there is a commutation relation hiding in such a system as follows [5]:

Consider two particles in one dimensional space with positions  $x_i$  ( $i = 1, 2$ ) and momentum operators  $\hat{p}_i = -i\hbar\frac{\partial}{\partial x_i}$ . Then a commutation relation arises as

$$[x_1 - x_2, \hat{p}_1 + \hat{p}_2] = 0 \quad (1)$$

According to QM's principle, there may be a kind of common eigenstate having eigenvalues of these two commutative (*i.e.*, compatible)observables like:

$$p_1 + p_2 = 0, (p_2 = -p_1) \quad \text{and} \quad (x_1 - x_2) = D \quad (2)$$

with  $D$  being their distance. The existence of such kind of eigenstate described by Eq.(2) puzzled Guan, he asked: "How can such kind of quantum state be realized?" A discussion between Guan and one of present authors (Ni) in 1998 led to a paper [6].

Here we are going to discuss further, showing that the correlation experiment on a  $K^0\bar{K}^0$  system (which just realized an entangled state composed of two spinless particles) in 1998 by CPLEAR collaboration [2] actually revealed some important features of QM and then answered the puzzle raised by EPR in a surprising way. First, besides Eq.(1), let us consider another three commutation relations simultaneously:

$$[t_1 + t_2, \hat{E}_1 - \hat{E}_2] = 0 \quad (3)$$

$$[x_1 + x_2, \hat{p}_1 - \hat{p}_2] = 0 \quad (4)$$

$$[t_1 - t_2, \hat{E}_1 + \hat{E}_2] = 0 \quad (5)$$

( $E_i = i\hbar \frac{\partial}{\partial t_i}$  with  $t_i$  being the time during which the  $i$ 'th particle is detected). In accordance with Ref.[2], we also focus on back-to-back events. The evolution of  $K^0 \bar{K}^0$ 's wavefunction (WF) will be considered in three inertial frames: The center-of-mass system  $S$  is at rest in laboratory with its origin  $x = 0$  located at the apparatus' center, where the antiprotons' beam is stopped inside a hydrogen gas target to create  $K^0 \bar{K}^0$  pairs by  $p\bar{p}$  annihilation. The  $K^0 \bar{K}^0$  pairs are detected by a cylindrical tracking detector located inside a solenoid providing a magnetic field parallel to the antiprotons' beam. For back-to-back events, the space-time coordinates in Eqs.(1)-(5) refer to particles moving to the right ( $x_1 > 0$ ) and left ( $x_2 < 0$ ) respectively. Second, we take an inertial system  $S'$  with its origin located at particle 1 (*i.e.*,  $x'_1 = 0$ ).  $S'$  is moving in a uniform velocity  $v$  with respect to  $S$ . (For Kaon's momentum of  $800 \text{ MeV}/c$ ,  $\beta = v/c = 0.849$ ). Another  $S''$  system is chosen with its origin located at particle 2 ( $x''_2 = 0$ ).  $S''$  is moving in a velocity  $(-v)$  with respect to  $S$ . Thus we have Lorentz transformation among the space-time coordinates being

$$\begin{cases} x' = \frac{x - vt}{\sqrt{1 - \beta^2}}, \\ t' = \frac{t - vx/c^2}{\sqrt{1 - \beta^2}}, \end{cases} \quad \begin{cases} x'' = \frac{x + vt}{\sqrt{1 - \beta^2}}, \\ t'' = \frac{t + vx/c^2}{\sqrt{1 - \beta^2}}, \end{cases} \quad (6)$$

Here  $t'_1$  and  $t''_2$  correspond to the proper time  $t_a$  and  $t_b$  in Ref.[2] respectively. The common time origin  $t = t' = t'' = 0$  is adopted.

A  $K^0 \bar{K}^0$  pair, created in a  $J^{PC} = 1^{--}$  antisymmetric state, can be described by a two-body WF depending on time as ([2], see also [7, 8])

$$\begin{aligned} |\Psi(0, 0)\rangle^{(antisym)} &= \frac{1}{\sqrt{2}} [ |K^0(0)\rangle_a |\bar{K}^0(0)\rangle_b - |\bar{K}^0(0)\rangle_a |K^0(0)\rangle_b ] \\ |\Psi(t_a, t_b)\rangle^{(antisym)} &= \frac{1}{\sqrt{2}} [ |K_S(0)\rangle_a |K_L(0)\rangle_b e^{-i(\alpha_S t_a + \alpha_L t_b)} - |K_L(0)\rangle_a |K_S(0)\rangle_b e^{-i(\alpha_L t_a + \alpha_S t_b)} ] \end{aligned} \quad (7)$$

with

$$|K_S\rangle = \frac{1}{\sqrt{2}} [|K^0\rangle - |\bar{K}^0\rangle], \quad |K_L\rangle = \frac{1}{\sqrt{2}} [|K^0\rangle + |\bar{K}^0\rangle] \quad (8)$$

where the CP violation has been neglected and  $\alpha_{S,L} = m_{S,L} - i\gamma_{S,L}/2$ ,  $m_{S,L}$  and  $\gamma_{S,L}$  being the  $K_{S,L}$  masses and decay widths, respectively. From Eq.(7), the intensities of events with like-strangeness ( $K^0 K^0$  or  $\bar{K}^0 \bar{K}^0$ ) and unlike-strangeness ( $K^0 \bar{K}^0$  or  $\bar{K}^0 K^0$ ) can be evaluated

as

$$I_{like}^{(antisy)}(t_a, t_b) = \frac{1}{8} e^{-2\gamma\tilde{t}} \{e^{-\gamma_S|t_a-t_b|} + e^{-\gamma_L|t_a-t_b|} - 2e^{-\gamma|t_a-t_b|} \cos[\Delta m(t_a - t_b)]\} \quad (9)$$

$$I_{unlike}^{(antisy)}(t_a, t_b) = \frac{1}{8} e^{-2\gamma\tilde{t}} \{e^{-\gamma_S|t_a-t_b|} + e^{-\gamma_L|t_a-t_b|} + 2e^{-\gamma|t_a-t_b|} \cos[\Delta m(t_a - t_b)]\} \quad (10)$$

where  $\Delta m = m_L - m_S$ ,  $\gamma = (\gamma_S + \gamma_L)/2$  and  $\tilde{t} = t_a$  (for  $t_a < t_b$ ) or  $\tilde{t} = t_b$  (for  $t_a > t_b$ ).

Similarly, for  $K^0 \bar{K}^0$  created in a  $J^{PC} = 0^{++}$  or  $2^{++}$  symmetric state as:

$$\begin{aligned} |\Psi(0, 0)\rangle^{(sym)} &= \frac{1}{\sqrt{2}} [ |K^0(0)\rangle_a |\bar{K}^0(0)\rangle_b + |\bar{K}^0(0)\rangle_a |K^0(0)\rangle_b ] \\ |\Psi(t_a, t_b)\rangle^{(sym)} &= \frac{1}{\sqrt{2}} [ |K_L(0)\rangle_a |K_L(0)\rangle_b e^{-i(\alpha_L t_a + \alpha_L t_b)} - |K_S(0)\rangle_a |K_S(0)\rangle_b e^{-i(\alpha_S t_a + \alpha_S t_b)} ] \end{aligned} \quad (11)$$

the predicted intensities read

$$\begin{aligned} I_{like}^{(sym)}(t_a, t_b) &= \frac{1}{8} \{e^{-\gamma_S(t_a+t_b)} + e^{-\gamma_L(t_a+t_b)} - 2e^{-\gamma(t_a+t_b)} \cos[\Delta m(t_a + t_b)]\} \\ I_{unlike}^{(sym)}(t_a, t_b) &= \frac{1}{8} \{e^{-\gamma_S(t_a+t_b)} + e^{-\gamma_L(t_a+t_b)} + 2e^{-\gamma(t_a+t_b)} \cos[\Delta m(t_a + t_b)]\} \end{aligned} \quad (12)$$

The experiment [2] reveals that the  $K^0 \bar{K}^0$  pairs are mainly created in the antisymmetric state shown by Eqs.(9)-(10) while the contribution in a symmetric state shown by Eqs.(11)-(12) accounts for 7.4%.

What we learn from Ref.[2] in combination with Eqs.(1)-(5) are as follows:

(a) Because only back-to-back events are involved in the  $S$  system, we denote three commutative operators as: the "distance" operator  $\hat{D} = x_1 - x_2 = v(t_1 + t_2)$ ,  $\hat{A} = \hat{p}_1 + \hat{p}_2$  and  $\hat{B} = \hat{E}_1 - \hat{E}_2$ , Eqs.(1) and (3) read

$$[\hat{D}, \hat{A}] = 0, [\hat{D}, \hat{B}] = 0, [\hat{A}, \hat{B}] = 0 \quad (13)$$

So they may have a kind of common eigenstate composed of  $K^0 \bar{K}^0$  in the symmetric state shown by Eq.(11) assigned by a continuous eigenvalue  $D_j = v(t_1 + t_2)$  (with continuous index  $j$ ) of operator  $\hat{D}$  as

$$\hat{D} |K^0 \bar{K}^0(sym)\rangle_j = D_j |K^0 \bar{K}^0(sym)\rangle_j = v(t_1 + t_2) |K^0 \bar{K}^0(sym)\rangle_j \quad (14)$$

$$\hat{A} |K^0 \bar{K}^0(sym)\rangle_j = A_j^{like} |K^0 \bar{K}^0(sym)\rangle_j = (p_1 + p_2) |K^0 \bar{K}^0(sym)\rangle_j \quad (15)$$

$$\hat{B} |K^0 \bar{K}^0(sym)\rangle_j = B_j^{like} |K^0 \bar{K}^0(sym)\rangle_j = (E_1 - E_2) |K^0 \bar{K}^0(sym)\rangle_j \quad (16)$$

where the lowest eigenvalue of  $\hat{A}$  is  $A_j^{like} = p_1 + p_2 = 0$ , ( $p_2 = -p_1$ ), and that of  $\hat{B}$  is  $B_j^{like} = E_1 - E_2 = 0$ , ( $E_2 = E_1$ ) respectively. These eigenstates of like-strangeness events predicted by Eq.(11) are really observed in the experiment [2] (these eigenstates of  $K^0\bar{K}^0$  were overlooked in the Ref.[6]).

(b) The more interesting case occurs for  $K^0\bar{K}^0$  pair created in the antisymmetric state with intensity given by Eq.(10) being a function of  $(t_a - t_b)$  (not  $(t_a + t_b)$  as shown by Eq.(12) for symmetric states) which is proportional to  $(t_1 - t_2)$  in the  $S$  system. In the EPR limit  $t_1 = t_2$ ,  $K^0\bar{K}^0$  events dominate whereas like-strangeness events are strongly suppressed as shown by Eq.(9) (see Fig.1 in [2]). So the experimental facts remind us of the possibility that  $K^0\bar{K}^0$  events may be related to common lowest (zero) eigenvalues of some commutative operators (just like what happened in Eqs.(15) and (16) for operators  $\hat{A}$  and  $\hat{B}$  [which are applied to symmetric states (due to  $\hat{D} = x_1 - x_2 = v(t_1 + t_2)$ ) but are not suitable for antisymmetric states], there are another three operators shown by Eqs.(4) and (5) being: the operator of "flight-path difference"  $\hat{F} = x_1 + x_2 = v(t_1 - t_2)$ ,  $\hat{M} = \hat{p}_1 - \hat{p}_2$  and  $\hat{G} = \hat{E}_1 + \hat{E}_2$  with commutation relations as:

$$[\hat{F}, \hat{M}] = 0, [\hat{F}, \hat{G}] = 0, [\hat{M}, \hat{G}] = 0 \quad (17)$$

which are just suitable for antisymmetric states. For  $K^0\bar{K}^0$  back-to-back events, assume that one of two particles, say 2, is an antiparticle with its momentum and energy operators being

$$\hat{p}_x^c = i\hbar \frac{\partial}{\partial x}, \quad \hat{E}^c = -i\hbar \frac{\partial}{\partial t} \quad (18)$$

(the superscript  $c$  means "antiparticle") just opposite in the sign to that for a particle. For instance, a freely moving particle's WF reads[\*]:

$$\psi(x, t) \sim \exp \left[ \frac{i}{\hbar} (px - Et) \right] \quad (19)$$

whereas

$$\psi_c(x, t) \sim \exp \left[ -\frac{i}{\hbar} (p_c x - E_c t) \right] \quad (20)$$

for its antiparticle with  $p_c$  and  $E_c (> 0)$  being momentum and energy of the antiparticle in accordance with Eq.(18). If using Eqs.(18)-(20), we find

$$\hat{F}|K^0\bar{K}^0(antisy)\rangle_k = F_k^{unlike}|K^0\bar{K}^0(antisy)\rangle_k = v(t_1 - t_2)|K^0\bar{K}^0(antisy)\rangle_k \quad (21)$$

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[\*] Please see the derivation of Eqs.(19) and (20) from the quantum field theory (QFT) at Eqs.(110)-(112).

with continuous index  $k$  referring to continuous eigenvalues  $F_k = v(t_1 - t_2)$ .

Now we use  $\hat{M}(=\hat{p}_1 - \hat{p}_2) = \hat{p}_1 + \hat{p}_2^c$  on  $K^0 \bar{K}^0$  system, yielding

$$\hat{M}|K^0 \bar{K}^0(antisy)\rangle_k = M_k^{unlike}|K^0 \bar{K}^0(antisy)\rangle_k = (p_1 + p_2^c)|K^0 \bar{K}^0(antisy)\rangle_k \quad (22a)$$

which means that the WF in space-time of this system reads

$$\langle x_1, t_1; x_2, t_2 | K^0 \bar{K}^0(antisy) \rangle \sim \Psi_{K^0 \bar{K}^0}^{antisy}(x_1, t_1; x_2, t_2) \sim [e^{i(p_1 x_1 - E_1 t_1)} \otimes e^{-i(p_2^c x_2 - E_2^c t_2)}]_{antisy} \quad (22b)$$

with antiparticle 2 moving opposite to particle 1 and  $p_2^c = -p_1$ . Similarly, we have

$$\hat{G}|K^0 \bar{K}^0(antisy)\rangle_k = G_k^{unlike}|K^0 \bar{K}^0(antisy)\rangle_k = (E_1 - E_2^c)|K^0 \bar{K}^0(antisy)\rangle_k \quad (23)$$

Hence we see that once Eqs.(18) and (20) are accepted, the states  $|K^0 \bar{K}^0(antisy)\rangle_k$  show up in experiments as the only states with strongest intensity at the EPR limit ( $t_1 = t_2$ ) corresponding to their three eigenvalues being all zero:  $F_k = M_k^{unlike} = G_k^{unlike} = 0$  and they won't change even when accelerator's energies are going up.

If using Eq.(18), the eigenvalues of  $\hat{A}$  and  $\hat{B}$  for the state  $|K^0 \bar{K}^0(sym)\rangle_j$  are  $A_j^{unlike} = p_1 - p_2^c = 2p_1$  and  $B_j^{unlike} = E_1 + E_2^c = 2E_1$  respectively, while that of  $\hat{M}$  and  $\hat{G}$  for the state  $|K^0 \bar{K}^0(antisy)\rangle_k$  are  $M_k^{like} = p_1 - p_2 = 2p_1$  and  $G_k^{like} = E_1 + E_2 = 2E_1$ , respectively, those eigenvalues are much higher than zero and going up with the accelerator's energy.

Something is very interesting here: If we deny Eq.(18) but insist on unified operators  $\hat{p}$  and  $\hat{E}$  for both particle and antiparticle, there would be no difference in eigenvalues between like-strangeness states and unlike-strangeness ones. For example, the  $M_k^{unlike}$  and  $G_k^{unlike}$  would be  $2p_1$  and  $2E_1$  too (instead of "0" as in Eqs.(18) and (23)). This would mean that three commutative operators  $\hat{F}$ ,  $\hat{M}$  and  $\hat{G}$  are not enough to distinguish the state  $|K^0 \bar{K}^0(antisy)\rangle_k$  from the state  $|K^0 K^0(antisy)\rangle_k$  even they behave so differently as shown by Eqs.(9) and (10), especially at the EPR limit ( $t_1 = t_2$ ).

Eq.(18) together with the identification of state  $|K^0 \bar{K}^0(antisy)\rangle_k$  by three zero eigenvalues implies that the difference of a particle from its antiparticle is not something hiding in the "intrinsic space" like opposite charge (for electron and positron) or opposite strangeness (for  $K^0$  and  $\bar{K}^0$ ) but can be displayed in their WFs evolving in space-time at the level of QM. To our knowledge, Eq.(18) can be found at a page note of a paper by Konopinski and Mahmaud in 1953 [9], also appears in Refs.[6, 10–13].

### III. WHAT IS THE ESSENCE OF CPT INVARIANCE?

There are three discrete transformations in quantum mechanics ( $QM$ ), quantum field theory ( $QFT$ ) and particle physics, see Refs.[7, 15, 16]

(a) Space-inversion ( $P$ ):

The sign change of space coordinates ( $\mathbf{x} \rightarrow -\mathbf{x}$ ) in the wave function ( $WF$ ) of  $QM$  may lead to two eigenstates:

$$\psi_{\pm}(\mathbf{x}, t) \rightarrow \psi_{\pm}(-\mathbf{x}, t) = \pm \psi_{\pm}(\mathbf{x}, t) \quad (24)$$

with eigenvalues 1 or  $-1$  being the even or odd parity.

(b) Time reversal ( $T$ ):

The so-called  $T$  transformation is actually not a "time reversal" but a "reversal of motion" [11, 16], which implies an antiunitary operator acting on the  $WF$ :

$$\psi(\mathbf{x}, t) \rightarrow \psi^*(\mathbf{x}, -t) \quad (25)$$

(c) Charge conjugation transformation( $C$ ):

The  $C$  transformation brings a particle (with charge  $q$ ) into its antiparticle (with charge  $-q$ ) and implies a complex conjugation on the  $WF$ :

$$\psi(\mathbf{x}, t) \rightarrow \psi_c(\mathbf{x}, t) \sim \psi^*(\mathbf{x}, t) \quad (26)$$

where the equivalence notation  $\sim$  possibly means some matrices in front of  $WF$  being ignored. Note that the  $WF$   $\psi_c$  implies a negative-energy particle. Usually, one has to resort to so-called "hole theory" for electron — the vacuum is fully filled with infinite negative-energy electrons and a "hole" created in the "sea" would correspond to a positron[15, 17]. But how could the "hole theory" be applied to the boson particle? No one knows.

(d)  $CPT$  combined transformation

If taking the product of  $C$ ,  $P$  and  $T$  transformations together, the complex conjugation contained in the  $C$  and  $T$  will cancel each other, yielding [7, 17]

$$\psi(\mathbf{x}, t) \rightarrow CPT\psi(\mathbf{x}, t) = \psi_{CPT}(\mathbf{x}, t) \sim \psi(-\mathbf{x}, -t) \quad (27)$$

On the right-hand-side (RHS), the  $WF$  should be understood as to describe an antiparticle. But it differs from the original  $WF$  only in the sign change of  $\mathbf{x}$  and  $t$ . What does it mean?

The historical discovery of parity violation in 1956-1957[18, 19] reveals that both  $P$  and  $C$  symmetries are violated in weak interactions. Since 1964, it is found that  $CP$  symmetry is also violated whereas the  $CPT$  invariance remains valid[\*], which in turn implies the

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[\*] It is verified mainly by the equality of the masses and lifetimes of a particle and its antiparticle, see [7, 20]

violation of  $T$  reversal symmetry, as summarized in the Review of Particle Physics [20].

Therefore, the relation between a particle  $|a\rangle$  and its antiparticle  $|\bar{a}\rangle$  is not  $|\bar{a}\rangle = C|a\rangle$  but (as defined by Lee and Wu[21])

$$|\bar{a}\rangle = CPT|a\rangle \quad (28)$$

which means exactly the Eq.(27). For example, for an electron in free motion, its  $WF$  reads

$$\langle \mathbf{x}, t | e^-, \mathbf{p}, E \rangle = \psi_{e^-}(\mathbf{x}, t) \sim \exp \left[ \frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{x} - Et) \right] \quad (29)$$

while the  $WF$  for a positron is given by Eq.(27) or Eq.(28) as

$$\langle \mathbf{x}, t | e^+, \mathbf{p}, E \rangle = \psi_{e^+}(\mathbf{x}, t) \sim \exp \left[ -\frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{x} - Et) \right] \quad (30)$$

Note that the momentum  $\mathbf{p}$  and energy  $E (> 0)$  are the same in Eqs.(29) and (30) (see Eq.(16.51) in [7]).

The above relation looks like a new symmetry: The (newly defined) space-time inversion ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) is equivalent to particle-antiparticle transformation. The transformation of a particle to its antiparticle (denoted by  $\mathcal{C}$ ) is not something which can be defined independently but a direct consequence of the (newly defined) space-time inversion  $\mathcal{PT}$  ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ )[10, 11, 22]:

$$\mathcal{PT} = \mathcal{C} \quad (31)$$

Now we see that the postulate, Eq.(31) is precisely in conformity with Eq.(18) versus

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \quad \hat{E} = i\hbar \frac{\partial}{\partial t} \quad (32)$$

for a particle. In other words, the symmetry between Eqs.(18) and (32) provides a concrete form of the postulate Eq.(31) at the QM level and it has been hinted strongly by the  $K^0 \bar{K}^0$  correlation experiment [2].

Some of our readers might still feel uncomfortable with the new particle-antiparticle transformation  $\mathcal{C}$  whose definition just resides in the postulate Eq.(31). To explain this, we should notice an important difference between a "theorem" and a "law" (or "postulate" before it can be well accepted). Various quantities contained in a theorem must be defined clearly and unambiguously in advance before the theorem can be proved. On the other hand, a law can often (not always) accommodate a definition of a physical quantity which can only be defined unambiguously after the law is verified by experiments. Two examples in classical physics are:



The definition of inertial mass  $m$  is contained in the Newton's dynamical law:

$$\mathbf{F} = m\mathbf{a} \quad (33)$$

The definition of electric (magnetic) field strength  $\mathbf{E}$  ( $\mathbf{B}$ ) is contained in the Lorentz-force formula:

$$\mathbf{F} = m \frac{d\mathbf{v}}{dt} = q \left( \mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \quad (34)$$

However, the definition of mass  $m$  in Eq.(33) ceases to be satisfying after the establishment of the theory of special relativity (SR) and QM. This is because the meaning and observableness of the force  $\mathbf{F}$  and acceleration  $\mathbf{a}$  in Eq.(33) become ambiguous to some extent. So nowadays, the definition of mass  $m$  is contained in the law of SR as

$$E^2 = p^2 c^2 + m^2 c^4 \quad (35)$$

for a freely moving particle, or simpler but better, given by the epoch-making discovery of Einstein

$$m = E/c^2 \quad (36)$$

for a rest particle [23]. The reason is: once a physical quantity (like the force  $\mathbf{F}$ ) lost its firm connection to a law, it ceases to be an observable and meaningful quantity in physics. By contrast, the energy  $E$  and momentum  $\mathbf{p}$  exhibit themselves as direct physical observables just because they obey a conservation law respectively.

The above words are also pertinent to a transformation in physics. When the  $C$ ,  $P$  and  $T$  transformations were introduced individually, they were based on the belief that they are valid in the nonrelativistic QM (NRQM) but had difficulties separately as mentioned above. Over time, when NRQM evolved into RQM and then QFT, physicists have been deliberately implementing these three discrete transformations in the Fock space for keeping their properties separately as follows (see [7, 14])

$P$ : particle unchanged but its momentum  $\mathbf{p} \rightarrow -\mathbf{p}$  and its spin component along some direction, say  $z$  axis,  $S_z$  remains unchanged.

$T$ : particle unchanged but  $\mathbf{p} \rightarrow -\mathbf{p}$ ,  $S_z \rightarrow -S_z$  and the direction of process is reversed in time.

$C$ : particle  $\rightarrow$  antiparticle, but their  $\mathbf{p}$ ,  $S_z$  and the direction of process remain unchanged.

Following the Eq.(16.51) in Ref.[7] we consider a real process as an example to show these transformations together with our postulate, Eq.(31).

The negative pion  $\pi^-(0)$  in its rest frame (with zero momentum) decays into a muon  $\mu^-$  and  $\bar{\nu}_\mu$  (or  $e^-$  and  $\bar{\nu}_e$ ). After 1957, all experiments (especially the GGS experiment in 1958, Ref.[24]) verify that neutrinos are left-handed polarized (so denoted by  $\nu_L$  regardless of their flavor) whereas antineutrinos are right-handed polarized ( $\bar{\nu}_R$ ). So we begin with the following process ( $\mathbf{p}$  is along  $z$  axis)

$$\pi^-(0) \rightarrow \mu_R^-(-\mathbf{p}, S_z = -1/2) + \bar{\nu}_R(\mathbf{p}, S_z = 1/2) \quad (37)$$

showing that both momentum and angular momentum are conserved.

After each transformation is performed on Eq.(37), the resulting process is shown in Eqs.(38)-(44) with  $(\checkmark)$  or  $(\times)$  referred to being "allowed" or "forbidden" in nature.

$$P : \pi^-(0) \rightarrow \mu_L^-(-\mathbf{p}, S_z = -1/2) + \bar{\nu}_L(\mathbf{p}, S_z = 1/2) \quad (\times) \quad (38)$$

$$C : \pi^+(0) \rightarrow \mu_R^+(-\mathbf{p}, S_z = -1/2) + \nu_R(\mathbf{p}, S_z = 1/2) \quad (\times) \quad (39)$$

$$T : \mu_R^-(\mathbf{p}, S_z = 1/2) + \bar{\nu}_R(-\mathbf{p}, S_z = -1/2) \rightarrow \pi^-(0) \quad (\checkmark) \quad (40)$$

$$CP : \pi^+(0) \rightarrow \mu_L^+(\mathbf{p}, S_z = -1/2) + \nu_L(-\mathbf{p}, S_z = 1/2) \quad (\checkmark) \quad (41)$$

$$PT : \mu_L^-(-\mathbf{p}, S_z = 1/2) + \bar{\nu}_L(\mathbf{p}, S_z = -1/2) \rightarrow \pi^-(0) \quad (\times) \quad (42)$$

$$CT : \mu_R^+(\mathbf{p}, S_z = 1/2) + \nu_R(-\mathbf{p}, S_z = -1/2) \rightarrow \pi^+(0) \quad (\times) \quad (43)$$

$$CPT : \mu_L^+(-\mathbf{p}, S_z = 1/2) + \nu_L(\mathbf{p}, S_z = -1/2) \rightarrow \pi^+(0) \quad (\checkmark) \quad (44)$$

$$\mathcal{PT} = \mathcal{C} : \mu_L^+(-\mathbf{p}, S_z = 1/2) + \nu_L(\mathbf{p}, S_z = -1/2) \rightarrow \pi^+(0) \quad (\checkmark) \quad (45)$$

The reason why processes (38),(39),(42) and (43) are forbidden is because  $\bar{\nu}_L$  or  $\nu_R$  doesn't exist in nature — this is so-called parity violation to its maximum. And the reason why the  $P$  and  $C$  transformations are violated in weak interactions is because their definitions are dividing the space-time from a particle's "intrinsic property" artificially —  $P$  only means the inversion in space whereas  $C$  "turns" a particle into its antiparticle without any change occurred to their WFs in the space-time. The maximal  $P$  and  $C$  violations in processes involving neutrinos remind us that nature doesn't work that way.

Hence though all discussions about  $P, C, CP$  or  $T$  transformations remain meaningful in cases either they are conserved or violated in one way or another. But the fact that their violations happen in certain specific cases whereas the  $CPT$  invariance always remains valid does strongly hint that  $C, P$  and  $T$  are essentially linked together as the  $CPT$  invariance and can be expressed by a simpler postulate as Eq.(31) shown also by Eq.(45) via the example of pion decay.

Below we are going to show when  $\mathcal{PT} = \mathcal{C}$  operation is acting on Eq.(37), how it turns out to be Eq.(45), which is precisely the same result as Eq.(44).

Let us first consider Eq.(19) and Eq.(20) at the QM level. Remember that time  $t$  always evolves forward before and after the  $\mathcal{PT}(\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t)$  transformation. By performing this transformation on the (invisible) WF Eq.(19) theoretically, what we "see" is just the annihilation of a particle (with momentum  $\mathbf{p}$  and energy  $E$ ) and the creation of its antiparticle (with the same value of momentum  $\mathbf{p}_c = \mathbf{p}$  and energy  $E_c = E$ ). In the real process Eq.(37),  $\mu_R^-$  and  $\bar{\nu}_R$  are created later than the existence of  $\pi^-(0)$ . But after the  $\mathcal{PT}$  transformation, the existence of  $\mu_L^+$  and  $\nu_L$  occurs earlier than that of  $\pi^+(0)$ . Furthermore, since the particle's momentum doesn't change its direction under the  $\mathcal{PT}$  transformation, but the spin's rotation does, so the helicity changes its sign after the transformation (which will be proved in detail in the next section).

#### IV. FROM QM VIA RQM TO QFT

In this section, we will discuss briefly the key role played by the postulate, Eq.(31), in the evolution from nonrelativistic QM (NRQM) via RQM to QFT (see Chap. 9 in [11]).

Let us begin with the energy conservation law for a particle in classical mechanics:

$$E = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{x}) \quad (46)$$

Consider the rule promoting observables into operators:

$$E \rightarrow \hat{E} = i\hbar \frac{\partial}{\partial t}, \quad \mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla \quad (47)$$

and let Eq.(46) act on a wavefunction (WF)  $\psi(\mathbf{x}, t)$ , the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + V(\mathbf{x}) \psi(\mathbf{x}, t) \quad (48)$$

follows immediately. In mid 1920's, considering the kinematical relation for a particle in the theory of special relativity (SR):

$$(E - V)^2 = c^2 \mathbf{p}^2 + m^2 c^4 \quad (49)$$

and using Eq.(47) again, the Klein-Gordon (KG) equation was established as:

$$(i\hbar \frac{\partial}{\partial t} - V)^2 \psi(\mathbf{x}, t) = -c^2 \hbar^2 \nabla^2 \psi(\mathbf{x}, t) + m^2 c^4 \psi(\mathbf{x}, t) \quad (50)$$

For a free KG particle, its plane-wave solution reads:

$$\psi(\mathbf{x}, t) \sim \exp\left[\frac{i}{\hbar}(\mathbf{p} \cdot \mathbf{x} - Et)\right] \quad (51)$$

However, two difficulties arose:

(a) The energy  $E$  in Eq.(51) has two eigenvalues:

$$E = \pm \sqrt{c^2 \mathbf{p}^2 + m^2 c^4} \quad (52)$$

What the "negative energy" means?

(b) The continuity equation is derived from Eq.(50) as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (53)$$

where

$$\rho = \frac{i\hbar}{2mc^2} \left( \psi^* \frac{\partial}{\partial t} \psi - \psi \frac{\partial}{\partial t} \psi^* \right) - \frac{1}{mc^2} V \psi^* \psi \quad (54)$$

and

$$\mathbf{j} = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) \quad (55)$$

are the "probability density" and "probability current density" respectively. While the latter is the same as that derived from Eq.(48), Eq.(54) seems not positive definite and dramatically different from  $\rho = \psi^* \psi$  in Eq.(48).

In 1958, Feshbach and Villars [25] recast Eq.(50) into two coupled Schrödinger-like equations as:

$$\begin{cases} \left( i\hbar \frac{\partial}{\partial t} - V \right) \phi = mc^2 \phi - \frac{\hbar^2}{2m} \nabla^2 (\phi + \chi) \\ \left( i\hbar \frac{\partial}{\partial t} - V \right) \chi = -mc^2 \chi + \frac{\hbar^2}{2m} \nabla^2 (\phi + \chi) \end{cases} \quad (56)$$

where

$$\begin{cases} \phi = \frac{1}{2} \left[ \left( 1 - \frac{1}{mc^2} V \right) \psi + \frac{i\hbar}{mc^2} \dot{\psi} \right] \\ \chi = \frac{1}{2} \left[ \left( 1 + \frac{1}{mc^2} V \right) \psi - \frac{i\hbar}{mc^2} \dot{\psi} \right] \end{cases} \quad (57)$$

( $\dot{\psi} = \frac{\partial \psi}{\partial t}$ ). Interestingly, the "probability density", Eq.(54) can be recast into a difference between two positive-definite densities [6, 8]:

$$\rho = \phi^* \phi - \chi^* \chi \quad (58)$$

Consider a constant  $V = V_0 < E$  for a positive-energy ( $E > 0$ ) particle. From Eqs.(51),(57) and (58) we see  $\rho > 0$  because  $|\phi|^2 > |\chi|^2$ . But for a negative-energy ( $E < 0$ ) particle, we

will have  $\rho_{E<0} = |\phi|^2 - |\chi|^2 < 0$ ! What happens? It must hint an antiparticle. However, being a "probability density",  $\rho$  is not allowed to be negative. We already know from previous section that for a freely moving ( $V = 0$ ) particle with  $E > 0$ , its WF  $\psi$  transforms into its antiparticle's WF  $\psi_c$  via a space-time inversion ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) as:  $\psi \rightarrow \psi_c \sim \exp(\frac{i}{\hbar} E_c t)$ , ( $E \rightarrow E_c > 0$ ). Now we easily see from Eq.(57) that ( $V = 0$ )  $\phi \rightarrow \chi_c, \chi \rightarrow \phi_c$  with  $|\chi_c| > |\phi_c|$ . Then an antiparticle emerges with its WF being

$$\psi_c \sim \chi_c \sim \phi_c \sim \exp[-\frac{i}{\hbar}(\mathbf{p}_c \cdot \mathbf{x} - E_c t)], \quad (|\chi_c| > |\phi_c|) \quad (59)$$

with momentum  $\mathbf{p}_c$  along the same direction as  $\mathbf{p}$  of the particle (using Eq.(18) instead of (47)). Just like the Eq.(18), we need a new "probability density"  $\rho_c$  for antiparticle versus  $\rho$ , Eq.(54) for particle, also a new "probability current density"  $\mathbf{j}_c$  for antiparticle versus  $\mathbf{j}$ , Eq.(55) for particle. So we can define in general case (with limitation that  $V < E$ ) that Eq.(56) is invariant under the (newly defined) space-time inversion ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) as follows

$$\begin{cases} V(\mathbf{x}, t) \rightarrow V(-\mathbf{x}, -t) = -V(\mathbf{x}, t) = V_c(\mathbf{x}, t), \\ \psi(\mathbf{x}, t) \rightarrow \psi(-\mathbf{x}, -t) = \psi_c(\mathbf{x}, t), \\ \phi(\mathbf{x}, t) \rightarrow \phi(-\mathbf{x}, -t) = \chi_c(\mathbf{x}, t), \\ \chi(\mathbf{x}, t) \rightarrow \chi(-\mathbf{x}, -t) = \phi_c(\mathbf{x}, t) \end{cases} \quad (60)$$

together with

$$\rho \rightarrow \rho_c = \frac{i\hbar}{2mc^2}(\psi_c \dot{\psi}_c^* - \psi_c^* \dot{\psi}_c) + \frac{1}{mc^2} V \psi_c^* \psi_c = \chi_c^* \chi_c - \phi_c^* \phi_c \quad (61)$$

which is positive definite again due to  $|\chi_c|^2 > |\phi_c|^2$  as we see from

$$\begin{cases} \chi_c = \frac{1}{2} \left[ \left( 1 + \frac{1}{mc^2} V \right) \psi_c - \frac{i\hbar}{mc^2} \dot{\psi}_c \right] \\ \phi_c = \frac{1}{2} \left[ \left( 1 - \frac{1}{mc^2} V \right) \psi_c + \frac{i\hbar}{mc^2} \dot{\psi}_c \right] \end{cases} \quad (62)$$

Similarly, we have

$$\mathbf{j} \rightarrow \mathbf{j}_c = \frac{i\hbar}{2m}(\psi_c^* \nabla \psi_c - \psi_c \nabla \psi_c^*) \quad (63)$$

which, for  $V = 0$  case, means

$$\mathbf{j} = \frac{\mathbf{p}}{m} |\psi|^2 \rightarrow \mathbf{j}_c = \frac{\mathbf{p}_c}{m} |\psi_c|^2, \quad (V = 0) \quad (64)$$

with  $\mathbf{j}_c$  along the direction of  $\mathbf{p}_c$  as expected. Eq.(53) remains valid after the above transformation too. Thus we see that both the "probability density"  $\rho$  for a particle and  $\rho_c$  for an antiparticle should be positive definite before they can be normalized as expected:

$$\int \rho d^3x = \int \rho_c d^3x = 1 \quad (65)$$

Instead of space-time inversion Eq.(60), the postulate Eq.(31), *i.e.*, the symmetry between particle and antiparticle, can also be realized by the invariance of Eq.(56) under the "mass inversion" as follows

$$\begin{cases} m \rightarrow -m \\ V(\mathbf{x}, t) \rightarrow V(\mathbf{x}, t), \\ \psi(\mathbf{x}, t) \rightarrow \psi_c(\mathbf{x}, t), \\ \phi(\mathbf{x}, t) \rightarrow \chi_c(\mathbf{x}, t), \\ \chi(\mathbf{x}, t) \rightarrow \phi_c(\mathbf{x}, t) \end{cases} \quad (66)$$

Notice that, when  $m \rightarrow -m$ , we have  $p \rightarrow -p_c$  and  $E \rightarrow -E_c$  for a free particle because momentum and energy are proportional to the mass in SR. Furthermore, for a process, the mass inversion, like the space-time inversion, implies that the direction of the process is reversed as well.

The reason why  $V \rightarrow -V$  in the space-time inversion Eq.(60) whereas  $V \rightarrow V$  in the mass inversion Eq.(66) can be seen from the classical equation: The Lorentz force  $\mathbf{F}$  on a particle exerted by an external potential  $\Phi$  reads:  $\mathbf{F} = -\nabla V = -\nabla(q\Phi) = m\mathbf{a}$ . The acceleration  $\mathbf{a}$  of particle will change to  $-\mathbf{a}$  for its antiparticle based on two alternative explanations: either due to the inversion of charge  $q \rightarrow -q$  (*i.e.*,  $V \rightarrow -V$  but keeping  $m$  unchanged) or due to the inversion of mass  $m \rightarrow -m$  (but keeping  $V$  unchanged).

We wish to stress that the newly defined space-time inversion, Eq.(60), is by no means a pure inversion in space-time. Rather, it must be linked with the transformation of particle into antiparticle as demanded by Eq.(31) (so after the space-time inversion the subscript  $c$  must be added). According to our experience, the "mass inversion", Eq.(66), with the mass  $m$  at the right-hand side being the antiparticle's mass  $m_c = m > 0$ , means precisely the same postulate Eq.(31) and is comparatively easier to be performed for reflecting the equal existence of a particle and its antiparticle.

The reason why Feshbach-Villars' dissociation of KG equation, Eq.(56), is so important is because they unveiled a new point of view for us to see a particle as follows:

For a free KG particle (say,  $K^-$  meson) moving at a high speed  $v$ , its WF  $\psi \sim e^{-iEt}$  ( $E > 0$ ) is always composed of two fields,  $\phi$  and  $\chi$ , in confrontation as shown by Eqs.(56) and (57). Calculations (as can be seen from Eq.(57)) show that: as long as  $E > 0$ , then  $|\phi| > |\chi|$  and  $\rho > 0$ , so  $\phi$  dominates  $\chi$  and  $K^-$  remains as a particle. However, the amplitude of  $\chi$  increases with the increase of particle's energy  $E$ : when  $v \rightarrow 0, E \rightarrow m, |\chi| \rightarrow 0$ , but when  $E \rightarrow \infty, |\chi| \rightarrow |\phi|$ , the ratio between them reads:  $|\chi|/|\phi| = [1 - (1 - v^2/c^2)^{1/2}]/[1 + (1 - v^2/c^2)^{1/2}]$ . What does this mean? It seems to us that while  $\phi$  (hidden in  $\psi$ ) characterizes the particle's

property,  $\chi$  represents the hidden "antiparticle (say,  $K^+$ ) field" in the WF of this  $K^-$  particle. Indeed, in Eqs.(51) and (59), the WFs of particle (dominated by  $\phi$ ) and antiparticle (dominated by  $\chi_c$ ), their phase variations with respect to space-time (keeping the same values of momentum and energy) are just in opposite directions, meaning that the intrinsic tendencies of space-time evolution of  $\phi$  and  $\chi$  are also in opposite directions essentially (see Eq.(56) with  $V = 0$ ). Hence, even the  $\chi$  is in a subordinate position in a particle, it still strives to display itself as follows: On one hand,  $\chi$  holds  $\phi$  back from going forward in space, so the particle's velocity  $v$  has an upper limit value  $c$  when  $|\chi|$  approaches  $|\phi|$ . And during the "boosting" process of a particle's wave-packet, it shows the Lorentz contraction due to the entanglement between  $\phi$  and  $\chi$  (see calculation shown in Fig.9.5.1 of Ref.[11]). On the other hand, a clock attached to the particle will show the time dilatation effect in SR with the increase of velocity  $v$ . This is because, in some sense, the "intrinsic clock" of  $\phi(\chi)$  is running clockwise (anticlockwise). With the enhancement of  $\chi$ , the particle's clock, though still runs clockwise, tends to stop. Therefore, it seems to us that all SR effects of a particle could be calculated and understood by the existence and enhancement of "hidden antiparticle field"  $\chi$  inside [11].

Hence, following Pauli and Weisskopf [26], we believe that a spinless particle in nature can be described by KG equation. While its positive-energy solution ( $\sim e^{-iEt/\hbar}$ ,  $E > 0$ ) describes a particle (*e.g.*,  $K^-$ ), its negative-energy solution ( $\sim e^{iEt/\hbar}$ ,  $E > 0$ ) should directly describe its antiparticle (*e.g.*,  $K^+$ ). What we add here is to emphasize their WFs linked by space-time inversion and the necessity of Eq.(47) versus (18). Eq.(56) throughout Eq.(66) are precisely showing the consistency of KG theory with our new point of view even at the QM level.

In this way, the Klein paradox [27] can be explained for KG equation. Please see Appendix.

At the level of QFT, the free "field operator" for a complex KG field and its hermitian conjugation are defined as ( $\hbar = c = 1$ )

$$\begin{cases} \hat{\psi}(\mathbf{x}, t) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2V\omega_{\mathbf{p}}}} \left\{ \hat{a}_{\mathbf{p}} \exp[i(\mathbf{p} \cdot \mathbf{x} - Et)] + \hat{b}_{\mathbf{p}}^{\dagger} \exp[-i(\mathbf{p} \cdot \mathbf{x} - Et)] \right\} \\ \hat{\psi}^{\dagger}(\mathbf{x}, t) = \sum_{\mathbf{p}} \frac{1}{\sqrt{2V\omega_{\mathbf{p}}}} \left\{ \hat{a}_{\mathbf{p}}^{\dagger} \exp[-i(\mathbf{p} \cdot \mathbf{x} - Et)] + \hat{b}_{\mathbf{p}} \exp[i(\mathbf{p} \cdot \mathbf{x} - Et)] \right\} \end{cases} \quad (67)$$

( $E = \omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2} > 0$ ) respectively. Here, after "field quantization", WFs' amplitudes have been promoted into  $\hat{a}_{\mathbf{p}}(\hat{b}_{\mathbf{p}})$  and  $\hat{a}_{\mathbf{p}}^{\dagger}(\hat{b}_{\mathbf{p}}^{\dagger})$  being the annihilation and creation operators for a particle (antiparticle) respectively.

In our opinion, being a basic postulate in QFT, the definition of field operator, Eq.(67), should respect the invariance of space-time inversion ( $\hat{\psi} \rightarrow \hat{\psi}, \hat{\psi}^\dagger \rightarrow \hat{\psi}^\dagger$ ), as long as a transformation of operators in Fock space is supplemented as [11, 28][\*]

$$\hat{a}_{\mathbf{p}} \leftrightarrow \hat{b}_{\mathbf{p}}^\dagger, \hat{a}_{\mathbf{p}}^\dagger \leftrightarrow \hat{b}_{\mathbf{p}} \quad (\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t \quad \text{or} \quad m \rightarrow -m) \quad (68)$$

Eqs.(67) and (68) imply that under the space-time (or mass) inversion, a process of particle's annihilation transforms into that of its antiparticle's creation (or vice versa), an ansatz could be understood intuitively in physics via discussions in the last section. So it seems to us that the present framework of QFT is well consistent with the new postulate, Eq.(31).

Let us turn to the Dirac equation describing an electron

$$\left( i\hbar \frac{\partial}{\partial t} - V \right) \psi = H\psi = (-i\hbar c \boldsymbol{\alpha} \cdot \nabla + \beta mc^2) \psi \quad (69)$$

with  $\boldsymbol{\alpha}$  and  $\beta$  being  $4 \times 4$  matrices, the WF  $\psi$  is a four-component spinor

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \quad (70)$$

Usually, the two-component spinors  $\phi$  and  $\chi$  are called "positive" and "negative" energy components. In our point of view, they are the hiding "particle" and "antiparticle" fields in a particle (electron) respectively ([11], see below). Substitution of Eq.(70) into Eq.(69) leads to

$$\begin{cases} \left( i\hbar \frac{\partial}{\partial t} - V \right) \phi = -i\hbar c \boldsymbol{\sigma} \cdot \nabla \chi + mc^2 \phi \\ \left( i\hbar \frac{\partial}{\partial t} - V \right) \chi = -i\hbar c \boldsymbol{\sigma} \cdot \nabla \phi - mc^2 \chi \end{cases} \quad (71)$$

( $\boldsymbol{\sigma}$  are Pauli matrices). Eq.(71) is invariant under the space-time inversion ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) with

$$\begin{cases} \phi(\mathbf{x}, t) \rightarrow \phi(-\mathbf{x}, -t) = \chi_c(\mathbf{x}, t), \quad \chi(\mathbf{x}, t) \rightarrow \chi(-\mathbf{x}, -t) = \phi_c(\mathbf{x}, t) \\ V(\mathbf{x}, t) \rightarrow V(-\mathbf{x}, -t) = -V(\mathbf{x}, t) = V_c(\mathbf{x}, t) \end{cases} \quad (72)$$

Note that under the space-time inversion, the  $\boldsymbol{\sigma}$  remain unchanged (However, see Eqs.(77)-(79) below). Alternatively, Eq.(71) also remains invariant under a mass inversion as

$$m \rightarrow -m, \quad \phi(\mathbf{x}, t) \rightarrow \chi_c(\mathbf{x}, t), \quad \chi(\mathbf{x}, t) \rightarrow \phi_c(\mathbf{x}, t), \quad V \rightarrow V \quad (73)$$

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[\*] Actually, this ansatz, Eq.(68), is contained in the proof of CPT theorem by Pauli [33], see the final section.



In either case of Eq.(72) or (73), we have[†]

$$\psi(\mathbf{x}, t) = \begin{pmatrix} \phi(\mathbf{x}, t) \\ \chi(\mathbf{x}, t) \end{pmatrix} \rightarrow \begin{pmatrix} \chi_c(\mathbf{x}, t) \\ \phi_c(\mathbf{x}, t) \end{pmatrix} = \psi'_c(\mathbf{x}, t) \quad (74)$$

For concreteness, we consider a free electron moving along the  $z$  axis with momentum  $p = p_z > 0$  and having a helicity  $h = \boldsymbol{\sigma} \cdot \mathbf{p}/|\mathbf{p}| = 1$ , its WF reads:

$$\psi(z, t) \sim \begin{pmatrix} \phi \\ \chi \end{pmatrix} \sim \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} \exp[i(p_z z - Et)] \quad (75)$$

with  $|\phi| > |\chi|$ . Under a space-time inversion ( $z \rightarrow -z, t \rightarrow -t, p \rightarrow p_c, E \rightarrow E_c$ ) or mass inversion ( $m \rightarrow -m, p \rightarrow -p_c, E \rightarrow -E_c$ ), it transforms into a WF for positron (moving along  $z$  axis)

$$\psi'_c(z, t) \sim \begin{pmatrix} \chi_c \\ \phi_c \end{pmatrix} \sim \begin{pmatrix} 1 \\ 0 \\ \frac{p_c}{E_c+m} \\ 0 \end{pmatrix} \exp[-i(p_c z - E_c t)] \quad (76)$$

with  $|\chi_c| > |\phi_c|$ , ( $p_c > 0, E_c > 0$ ). However, the positron's helicity becomes  $h_c = \boldsymbol{\sigma}_c \cdot \mathbf{p}_c/|\mathbf{p}_c| = -1$ . This is because the total angular momentum operator for an electron reads

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \frac{\hbar}{2} \boldsymbol{\sigma} \quad (77)$$

Under a space-time inversion, the orbital angular momentum operator transforms as

$$\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}} = \mathbf{r} \times (-i\hbar\nabla) \rightarrow -\mathbf{r} \times (i\hbar\nabla) = -\mathbf{r} \times \hat{\mathbf{p}}_c = -\hat{\mathbf{L}}_c \quad (78)$$

To get  $\hat{\mathbf{j}} \rightarrow -\hat{\mathbf{j}}_c$  with  $\hat{\mathbf{j}}_c = \hat{L}_c + \frac{\hbar}{2} \hat{\boldsymbol{\sigma}}_c$ , we should have

$$\hat{\boldsymbol{\sigma}}_c = -\hat{\boldsymbol{\sigma}} \quad (79)$$

Hence the values of matrix element for positron's spin operator  $\boldsymbol{\sigma}_c$  is just the negative to that for  $\boldsymbol{\sigma}$  in the same matrix representation.

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[†] The reason why we use  $\psi'_c$  instead of  $\psi_c$  will be clear in Eqs.(80)-(83). Actually, we emphasize Dirac equation as a coupling equation of two two-component spinors, Eq.(71), rather than merely a four-component spinor equation.

Thus we are able to clarify the helicity problem in Eq.(45) as follows: Eq.(75) describes an electron with positive helicity, *i.e.*,  $\mathbf{\Sigma} \cdot \hat{\mathbf{p}}\psi = p_z\psi = p\psi$  [†]. Under a space-time inversion, it transforms into  $(-\mathbf{\Sigma}_c) \cdot \hat{\mathbf{p}}_c\psi'_c = \Sigma_z(i\hbar\frac{\partial}{\partial z})\psi'_c = p_c\psi'_c$  in Eq.(76), *i.e.*,  $\mathbf{\Sigma}_c \cdot \hat{\mathbf{p}}_c\psi'_c = -p_c\psi'_c$ , meaning that Eq.(76) describes a positron with negative helicity.

Dirac equation is usually written in a covariant form as (Pauli metric is used:  $x_4 = ict$ ,  $\gamma_k = -i\beta\alpha_k$ ,  $\gamma_4 = \beta$ ,  $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 = -\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$ , see [15]):

$$(\gamma_\mu\partial_\mu + m)\psi = 0 \quad (80)$$

Under a space-time (or mass) inversion, it turns into an equation for antiparticle:

$$(-\gamma_\mu\partial_\mu + m)\psi'_c = 0 \quad (81)$$

with an example of  $\psi'_c$  shown in Eq.(76). Let us perform a representation transformation:

$$\psi'_c \rightarrow \psi_c = (-\gamma_5)\psi'_c = \begin{pmatrix} \phi_c \\ \chi_c \end{pmatrix} \quad (82)$$

and arrive at

$$(\gamma_\mu\partial_\mu + m)\psi_c = 0 \quad (83)$$

due to  $\{\gamma_5, \gamma_\mu\} = 0$ . Since  $\psi_c$  and  $\psi'_c$  are essentially the same in physics, (this is obviously seen from its resolved form, Eq.(71)), it is merely a trivial thing to change the position of  $\chi_c$  in the spinor (lower in Eq.(82) and upper in Eq.(76)). What important is  $|\chi_c| > |\phi_c|$  for characterizing an antiparticle versus  $|\phi| > |\chi|$  for a particle. Therefore, if a particle with energy  $E$  runs into a potential barrier  $V = V_0 > E + m$ , its WF's third component in Eq.(75) suddenly turns into  $\frac{p'}{E - V_0 + m} = \frac{-p'}{V_0 - E - m}$ , ( $p' = \sqrt{(E - V_0)^2 - m^2}$ ), whose absolute magnitude is larger than the first one. This means that it is an antiparticle's WF now (because  $|\chi| > |\phi|$ ) and will be crucial for the explanation of Klein paradox in Dirac equation as shown in the Appendix. However, we need to discuss the "probability density"  $\rho$  and "probability current density"  $\mathbf{j}$  for a Dirac particle versus  $\rho_c$  and  $\mathbf{j}_c$  for its antiparticle. Different from that in KG equation, now we have

$$\rho = \psi^\dagger\psi = \phi^\dagger\phi + \chi^\dagger\chi \rightarrow \rho_c = \psi_c^\dagger\psi_c = \chi_c^\dagger\chi_c + \phi_c^\dagger\phi_c \quad (84)$$

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[†]  $\mathbf{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}$ ,  $\mathbf{\Sigma}_c = \begin{pmatrix} \boldsymbol{\sigma}_c & 0 \\ 0 & \boldsymbol{\sigma}_c \end{pmatrix}$

which is positive definite for either particle or antiparticle. On the other hand, we have

$$\mathbf{j} = c\psi^\dagger \boldsymbol{\alpha} \psi = c(\phi^\dagger \boldsymbol{\sigma} \chi + \chi^\dagger \boldsymbol{\sigma} \phi) \rightarrow \mathbf{j}_c = c\psi_c^\dagger \boldsymbol{\alpha} \psi_c = c(\chi_c^\dagger \boldsymbol{\sigma} \phi_c + \phi_c^\dagger \boldsymbol{\sigma} \chi_c) \quad (85)$$

(we prefer to keep  $\boldsymbol{\sigma}$  rather than  $\boldsymbol{\sigma}_c$  for antiparticle). For Eqs.(75), (76) and (82), we find ( $c = \hbar = 1$ )

$$j_z \sim \frac{2p}{E+m} > 0 \rightarrow j_z^c \sim \frac{2p_c}{E_c+m} > 0 \quad (V=0) \quad (86)$$

which means that the probability current is always along the momentum's direction for either a particle or antiparticle. Besides  $\phi \rightarrow \chi_c, \chi \rightarrow \phi_c$  and so  $|\phi| > |\chi|$  but  $|\chi_c| > |\phi_c|$ , Eqs.(85)-(86) will also be a key criterion.

Above discussions at RQM level may be summarized as follows: The first symptom for the appearance of an antiparticle is: If we perform an energy operator ( $E = i\hbar\partial/\partial t$ ) on a WF and find a negative energy ( $E < 0$ ) or a negative kinetic energy ( $E - V < 0$ ), we'd better to doubt the WF being a description of antiparticle. Then for further confirmation, two more criterions are needed (see Appendix).

In hindsight, for a linear equation in RQM, either KG or Dirac equation, the emergence of both positive and negative energy ( $E$ ) WFs is inevitable and natural (just like the energy  $E' = E - mc^2$  in the NRQM must be both positive and negative). From mathematical point of view, the set of WFs cannot be complete if without taking the negative energy solutions into account. And physicists believe that these negative-energy solutions might be relevant to antiparticles. However, we physicists admit that both a rest particle's energy  $E = mc^2$  and a rest antiparticle's energy  $E_c = m_c c^2 = mc^2$  are positive, as verified by the experiments of pair-creation process  $\gamma \rightarrow e^+ + e^-$ . The above contradiction constructs so-called "negative-energy paradox" in RQM. For Dirac particle, majority (not all) of physicists accept the "hole theory" to explain the "paradox". But for KG particle, no such kind of "hole theory" can be acceptable. It was this "negative-energy paradox" and "Klein paradox" as well as the four "commutation relations", Eqs.(1)-(5), hidden in the two-particle system discussed by EPR [1] (and pointed out to us first by Guan[5]) gradually prompted us to realize that the root cause of difficulty in RQM lies in an a priori notion — only one kind of WF with one set of operators (like Eq.(47)) can be acceptable in QM, either for NRQM or RQM.

Once getting rid of the constraint in the above notion, we are able to see that many difficulties in RQM disappear immediately, based on two sets of WFs and operators for particle and antiparticle respectively and being linked together by Eq.(31).

At the QFT level, the "field operator" for Dirac field can be directly constructed in the following form (see Refs. [14, 15])

$$\begin{cases} \hat{\psi}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \sum_{h=\pm 1} \sqrt{\frac{m}{E}} \left[ \hat{a}_{\mathbf{p}}^{(h)} u^{(h)}(\mathbf{p}) e^{i(\mathbf{p} \cdot \mathbf{x} - Et)} + \hat{b}_{\mathbf{p}}^{(h)\dagger} v^{(h)}(\mathbf{p}) e^{-i(\mathbf{p} \cdot \mathbf{x} - Et)} \right] \\ \hat{\psi}^\dagger(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \sum_{h=\pm 1} \sqrt{\frac{m}{E}} \left[ \hat{a}_{\mathbf{p}}^{(h)\dagger} u^{(h)\dagger}(\mathbf{p}) e^{-i(\mathbf{p} \cdot \mathbf{x} - Et)} + \hat{b}_{\mathbf{p}}^{(h)} v^{(h)\dagger}(\mathbf{p}) e^{i(\mathbf{p} \cdot \mathbf{x} - Et)} \right] \end{cases} \quad (87)$$

Here for arbitrary momentum  $\mathbf{p}$  (with direction denoted by angles  $\theta$  and  $\phi$  in spherical coordinates) and energy  $E = \sqrt{\mathbf{p}^2 + m^2} > 0$ , the spinors attached to particle's annihilation operators  $\hat{a}_{\mathbf{p}}^{(h)}$  are

$$u^{(1)}(\mathbf{p}) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \phi_0^{(1)}(\mathbf{p}) \\ \frac{|\mathbf{p}|}{E+m} \phi_0^{(1)}(\mathbf{p}) \end{pmatrix}, \quad u^{(-1)}(\mathbf{p}) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \phi_0^{(-1)}(\mathbf{p}) \\ \frac{-|\mathbf{p}|}{E+m} \phi_0^{(-1)}(\mathbf{p}) \end{pmatrix} \quad (88)$$

$$\phi_0^{(1)}(\mathbf{p}) = \begin{pmatrix} \cos \theta/2 \\ e^{i\phi} \sin \theta/2 \end{pmatrix}, \quad \phi_0^{(-1)}(\mathbf{p}) = \begin{pmatrix} \sin \theta/2 \\ -e^{i\phi} \cos \theta/2 \end{pmatrix}, \quad u^{(h)\dagger}(\mathbf{p}) u^{(h')}(\mathbf{p}) = \frac{E}{m} \delta_{hh'} \quad (89)$$

while that attached to antiparticle's creation operators  $\hat{b}_{\mathbf{p}}^{(h)\dagger}$  are

$$v^{(h)}(\mathbf{p}) = (-\gamma_5) u^{(-h)}(\mathbf{p}), \quad (h = \pm 1) \quad (90)$$

$$v^{(h)\dagger}(\mathbf{p}) v^{(h')}(\mathbf{p}) = \frac{E}{m} \delta_{hh'}, \quad v^{(h')\dagger}(-\mathbf{p}) u^{(h)}(\mathbf{p}) = u^{(h')\dagger}(-\mathbf{p}) v^{(h)}(\mathbf{p}) = 0 \quad (91)$$

In our point of view, Eq.(87) respect the invariance of space-time inversion (up to a trivial representation transformation Eq.(82)),  $\hat{\psi} \rightarrow \hat{\psi}, \hat{\psi}^\dagger \rightarrow \hat{\psi}^\dagger$ , with the following ansatz similar to that for KG field (Eq.(68))

$$\hat{a}_{\mathbf{p}}^{(h)} \rightleftharpoons \hat{b}_{\mathbf{p}}^{(-h)\dagger}, \quad \hat{a}_{\mathbf{p}}^{(h)\dagger} \rightleftharpoons \hat{b}_{\mathbf{p}}^{(-h)}, \quad (\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t, \text{ or } m \rightarrow -m) \quad (92)$$

For either KG or Dirac field, no resort to "hole" theory is needed here. Of course, Eq.(87) with Eq.(92) is essentially a postulate, whose validity can only be verified via comparisons between QFT's predictions and experiments. But there is an argument accepted in particle physics as follows: Based on well known process of beta decay:  $n \rightarrow p + e^- + \bar{\nu}_e$ , one can move  $e^-$  from the right to left side (yielding  $n - e^- \rightarrow p + \bar{\nu}_e$ ) and then predict a real process as  $n + e^+ \rightarrow p + \bar{\nu}_e$ , implying the annihilation of  $e^-$  being "equivalent to" the creation of its antiparticle  $e^+$ . Here the words "equivalent to" could be better replaced by "transformed into ...under a space-time or mass inversion". [\*]

[\*] Hence we see that the operation of Eq.(31) can be performed in a rather flexible manner — it can either bring a whole process like Eq.(37) into Eq.(45), or just transforms one particle in a process like  $e^-$  in the beta decay into  $e^+$  here for predicting a new process. Another example is: In the Dirac equation for a hydrogenlike atom, Eq.(71), while the electron is transformed into a positron under the operation of Eq.(31), the nucleus remains unchanged at all (see Ref.[13]).

However, there are considerable differences between KG field and Dirac field. The annihilation and creation operators for KG particles obey commutation relations as

$$[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}^\dagger] = [\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}^\dagger] = \delta_{\mathbf{p}\mathbf{p}'}, [\hat{a}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = 0, \text{ etc.} \quad (93)$$

Also, instead of  $\rho$  (Eq.(58)) or  $\rho_c$  (Eq.(61)) at QM level, a "charge number" operator is defined for KG field at QFT level as (promoting  $\psi \rightarrow \hat{\psi}$  and  $\psi^* \rightarrow \hat{\psi}^\dagger$  in Eq.(54) with  $V = 0$  and a factor  $\frac{\hbar}{2mc^2}$  ignored)

$$\hat{Q}_{KG} \equiv i \int (\hat{\psi}^\dagger \frac{\partial}{\partial t} \hat{\psi} - \hat{\psi} \frac{\partial}{\partial t} \hat{\psi}^\dagger) d^3x = \sum_{\mathbf{p}} (\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} - \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}}) \quad (94)$$

where Eq.(93) had been used. For many-KG-particle system, the eigenvalue of  $\hat{Q}$ , called as the "charge number" (may be up to a sign), is conserved in natural processes.

On the other hand, at QM level, one Dirac particle (either electron or positron) always has a positive-definite "probability density":

$$\rho = \bar{\psi} \gamma_4 \psi = \psi^\dagger \psi = \phi^\dagger \phi + \chi^\dagger \chi \quad (95)$$

which does not change in form under a space-time inversion. However, at QFT level, because of anticommutation relations as

$$\{\hat{a}_{\mathbf{p}}^{(h)}, \hat{a}_{\mathbf{p}'}^{(h')\dagger}\} = \{\hat{b}_{\mathbf{p}}^{(h)}, \hat{b}_{\mathbf{p}'}^{(h')\dagger}\} = \delta_{\mathbf{p}\mathbf{p}'} \delta_{hh'}, \{\hat{a}_{\mathbf{p}}^{(h)}, \hat{b}_{\mathbf{p}'}^{(h')}\} = 0, \text{ etc.} \quad (96)$$

in contrast to Eq.(93), the "charge number" operator for Dirac field is similar to Eq.(94) for KG field

$$\hat{Q}_{Dirac} = \int \hat{\rho} d^3x = \int \hat{\psi}^\dagger \hat{\psi} d^3x = \sum_{\mathbf{p}, h} (\hat{a}_{\mathbf{p}}^{(h)\dagger} \hat{a}_{\mathbf{p}}^{(h)} - \hat{b}_{\mathbf{p}}^{(h)\dagger} \hat{b}_{\mathbf{p}}^{(h)}) \quad (97)$$

where a "normal order" had been used to eliminate an infinite constant. The eigenvalue of  $\hat{Q}$ , the "fermion number", is conserved in a multi-fermion system.

Note that the continuity equation Eq.(53) is at the QM level, not like that for the "electric charge  $q$ " at the level of classical electrodynamics in the 19th century. The "charge  $q$ " is no longer conserved as shown by the enhancement of the fine-structure-constant  $\alpha = e^2/\hbar c$  from 1/137 at low energy to 1/128 at high energy. Nowadays, what conserved is the "charge number"  $Q = q/e$  like that shown by Eqs.(94) and (97).

Moreover, just like a  $K^-$  meson moving at high speed discussed previously, a freely moving electron also has two hidden fields,  $\phi$  and  $\chi$ , in confrontation inside as shown by Eq.(75) with  $|\phi| > |\chi|$ . Being a "hidden positron field",  $\chi$ 's amplitude increases with the electron's velocity  $v$  and its ratio to  $\phi$ ,  $R = |\chi|/|\phi| = \{[1 - (1 - v^2/c^2)^{1/2}]/[1 + (1 - v^2/c^2)^{1/2}]\}^{1/2}$ ,

approaches 1. But as long as  $v < c$ ,  $R < 1$  and the electron remains as an electron, so is the charge number —  $Q = -1$  unchanged. The enhancement of  $\chi$  field never displays as some increasing "positive charge" to "neutralize" the overall negative charge of electron. On the contrary, the electron's charge (absolute value) even increases with its velocity as shown by the increasing value of  $\alpha$ .

Interestingly, if we (incorrectly) use the anticommutation (commutation) relations for KG (Dirac) field, we would have

$$\hat{Q}'_{KG} = \sum_{\mathbf{p}} (\hat{b}_{-\mathbf{p}} \hat{a}_{\mathbf{p}} - \hat{a}_{\mathbf{p}}^\dagger \hat{b}_{-\mathbf{p}}^\dagger) \quad (98)$$

and

$$\hat{Q}'_{Dirac} = \sum_{\mathbf{p}, h} (\hat{a}_{\mathbf{p}}^{(h)\dagger} \hat{a}_{\mathbf{p}}^{(h)} + \hat{b}_{\mathbf{p}}^{(h)\dagger} \hat{b}_{\mathbf{p}}^{(h)} + 1) \quad (99)$$

Both Eq.(98) and (99) are wrong. Hence we see that the correct spin-statistics connection is an indispensable and compatible ingredient in the evolution of theory from QM level to QFT level. [\*]

Furthermore, let us look at the key role played by the postulate Eq.(31) in the evolution of Green function in NRQM into that in RQM and QFT. In NRQM, the evolution of a particle's WF with time is described by Feynman as [11, 16, 28]

$$\psi(\mathbf{x}_b, t_b) = \int K(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) \psi(\mathbf{x}_a, t_a) d^3 x_a \quad (100)$$

$$K(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a) = \sum_{a \rightarrow b, \text{all paths}} \text{const.} \exp\left(\frac{i}{\hbar} S[\mathbf{x}(t)]\right) \quad (101)$$

with classical action  $S[\mathbf{x}(t)]$  being evaluated along a path connecting  $(\mathbf{x}_a, t_a)$  to  $(\mathbf{x}_b, t_b)$ . However, all paths, in spite of their arbitrariness, must go forward in time. This can also be seen from the Green function of Schrödinger equation

$$(i\hbar \frac{\partial}{\partial t} - \hat{H})G(\mathbf{x}, t | \mathbf{x}', t') = \delta(\mathbf{x} - \mathbf{x}') \delta(t - t') \quad (102)$$

$$G(\mathbf{x}, t | \mathbf{x}', t') = -\frac{i}{\hbar} K(\mathbf{x}, t | \mathbf{x}', t') \theta(t - t'), \quad \theta(t - t') = \begin{cases} 1, & t > t'; \\ 0, & t < t'. \end{cases} \quad (103)$$

Hence the Green function  $G$  given by Eq.(103) is essentially the same as the Feynman kernel function  $K$  defined by Eq.(101), except for the existence of  $\theta$  function showing explicitly that

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[\*] Interestingly, Peskin and Schroeder in their book ([14], §3.5A) discussed how an incorrect "field operator" (with  $\hat{b}_{\mathbf{p}}^{(h)}$  and  $\hat{b}_{\mathbf{p}}^{(h)\dagger}$  exchanged in Eq.(87)) and wrong "commutation relation" (instead of anticommutation relation, Eq.(96)) for Dirac field would lead us to a blind alley for QFT.

the reversal in time is not allowed. This reminds us once again of the "misnomer" of so-called "time-reversal" in NRQM as discussed in Section II. (To our knowledge, Sakurai first stressed this point in his book [16]).

The situation is dramatically different in RQM, where the Feynman propagator for electron,  $S_F(x - x')$ , is defined by

$$(\gamma_\mu \partial_\mu + m)S_F(x - x') = \delta^{(4)}(x - x') = -i\delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta(t - t') \quad (104)$$

$$S_F(x - x') = \sum_{\mathbf{p}, h} \frac{m}{EV} \left[ u^{(h)}(\mathbf{p}) \bar{u}^{(h)}(\mathbf{p}) e^{ip \cdot (x - x')} \theta(t - t') - v^{(h)}(\mathbf{p}) \bar{v}^{(h)}(\mathbf{p}) e^{-ip \cdot (x - x')} \theta(t' - t) \right] \quad (105)$$

It is equivalent to the two-point Green function of Dirac field in QFT

$$S_F(x - x') = \langle 0 | T \hat{\psi}(x) \bar{\hat{\psi}}(x') | 0 \rangle \quad (106)$$

where the vacuum state  $|0\rangle$  is defined by

$$\hat{a}_{\mathbf{p}}^{(h)} |0\rangle = \hat{b}_{\mathbf{p}}^{(h)} |0\rangle = 0 \quad (107)$$

The meaning of Eq.(106) can be seen from its matrix element with indices  $\alpha$  and  $\beta$ :

$$[S_F(x - x')]_{\alpha\beta} = \langle 0 | \hat{\psi}_\alpha(x) \bar{\hat{\psi}}_\beta(x') | 0 \rangle \theta(t - t') - \langle 0 | \bar{\hat{\psi}}_\beta(x') \hat{\psi}_\alpha(x) | 0 \rangle \theta(t' - t) \quad (108)$$

Usually, Eq.(108) is interpreted as follows: when  $t > t'$ , a virtual electron propagates from  $x'$  to  $x$ ; but when  $t' > t$ , a virtual positron goes from  $x$  to  $x'$ . Historically, the latter case was described by Stüekelberg in 1941 [29] as "a negative-energy electron going backward in time (from  $x'$  to  $x$  with  $t' > t$ )". This interpretation forms the basis of Feynman's space-time approach for QED ([30], see also [15]).

Let us perform a space-time inversion on Eq.(105):

$$\begin{aligned} S_F(x - x') &\rightarrow S_F(x' - x) = S_F^c(x - x') \\ &= \sum_{\mathbf{p}, h} \frac{m}{EV} \left[ u^{(h)}(\mathbf{p}) \bar{u}^{(h)}(\mathbf{p}) e^{-ip \cdot (x - x')} \theta(t' - t) - v^{(h)}(\mathbf{p}) \bar{v}^{(h)}(\mathbf{p}) e^{ip \cdot (x - x')} \theta(t - t') \right] \\ &= (-\gamma_5) S_F(x - x') (-\gamma_5) \sim S_F(x - x') \end{aligned} \quad (109)$$

which means that  $S_F(x - x')$  is invariant under the space-time inversion up to a trivial representation transformation.

To close this section, we wish to show that the WFs of particle and antiparticle, Eqs.(75) and (82), can also be derived from QFT as follows:

In QFT, the WF of a single particle should be defined rigorously as the nondiagonal matrix element of the relevant field operator between the vacuum state and one-particle state. For instance, assume Eq.(87) to be the "field operator for electron field", then the WF of a freely moving electron (with momentum  $\mathbf{p}_1$  and helicity  $h_1$ ) is given by

$$\psi_{e-}(\mathbf{x}, t) = \langle 0 | \hat{\psi}(\mathbf{x}, t) | e^-, \mathbf{p}_1, h_1 \rangle = \langle 0 | \hat{\psi}(\mathbf{x}, t) \hat{a}_{\mathbf{p}_1}^{(h_1)\dagger} | 0 \rangle = \frac{1}{\sqrt{V}} \sqrt{\frac{m}{E_1}} u^{(h_1)}(\mathbf{p}_1) e^{i(\mathbf{p}_1 \cdot \mathbf{x} - E_1 t)} \quad (110)$$

but the hermitian conjugate of a positron's WF is given by

$$\psi_{e+}^\dagger(\mathbf{x}, t) = \langle 0 | \hat{\psi}^\dagger(\mathbf{x}, t) | e^+, \mathbf{p}_c, h_c \rangle = \langle 0 | \hat{\psi}^\dagger(\mathbf{x}, t) \hat{b}_{\mathbf{p}_c}^{(h_c)\dagger} | 0 \rangle = \frac{1}{\sqrt{V}} \sqrt{\frac{m}{E_c}} v^{(h_c)\dagger}(\mathbf{p}_c) e^{i(\mathbf{p}_c \cdot \mathbf{x} - E_c t)} \quad (111)$$

which leads to positron's WF being

$$\psi_{e+}(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sqrt{\frac{m}{E_c}} v^{(h_c)}(\mathbf{p}_c) e^{-i(\mathbf{p}_c \cdot \mathbf{x} - E_c t)} \quad (112)$$

Eq.(110) and (112) are precisely the WFs at the level of RQM, Eq.(75) and (82), showing that the underlying symmetry, Eq.(31), runs through the RQM and QFT in a consistent way. To our knowledge and surprise, no such simple derivation like Eqs.(110)-(112) could be found in existing textbooks or literatures. As long as WFs for particle and antiparticle emerge unambiguously as Eqs.(110) and (112), two sets of operators at the level of RQM (like Eq.(18) versus Eq.(47), *etc.*) follow immediately.

## V. SUMMARY AND DISCUSSION

Thanks to pioneering works on the CPT theorem [31–34] and the delicate experimental tests for decades, the CPT invariance has been firmly established [20]. It seems to us that since the discovery of parity violation in 1956-1967, the CPT invariance has been gradually transforming itself into a basic postulate — the  $\mathcal{PT} = \mathcal{C}$  symmetry, Eq.(31). In some sense, we just look at the CPT theorem upside down. The reason is as follows.

A theorem in physics shares a common feature with the theorem in mathematics that their consequences are already hidden in their premises (which are beyond the proof of theorem itself). However, there is big difference here. For a theorem in mathematics, its premises are composed of axioms. For example, different axioms lead to different logic structures of geometry, either Euclidean or Riemanian. Both of them are correct in mathematics.



Einstein's choice of Riemann geometry (instead of Euclidean geometry) for inventing his theory of general relativity was not a judgement on mathematics but an inference from physics, *e.g.*, the correct prediction of solar deflection angle of light-ray from a distant star.

For a theorem (or in general, a theory) in physics, its premises are not something which can be chosen at physicists' disposal. Rather, the premises should be retrospected to fewest principles, or postulates, which cannot be proved or disproved by themselves (or by other existing theory) but should be verified or invalidated by experiments. For instance, the postulates of NRQM proposed by Heisenberg, or by Schrödinger, or Dirac, or Feynman are essentially equivalent despite of different expressions used (as can be proved by the theory), but the validity of NRQM must be verified by experiments. After the combination of NRQM with SR, the RQM was established and predicted the existence of antiparticles. Then the question is: What is the new postulate hidden in SR but had been essentially injected into NRQM for its evolution into RQM, QFT and particle physics? It seems to us that the new postulate was missed for a long time until discovered implicitly by Lüders [31, 32] and Pauli [33] via their proof of CPT theorem. As explained by Lüders [32], the CPT theorem claims that "a wide class of QFTs which are invariant under the proper Lorentz group is also invariant with respect to the product of  $T$ ,  $C$  and  $P$ ". The proof of CPT theorem contains a crucial step being the construction of so-called "strong reflection", consisting in a reflection of space and time about some arbitrarily chosen origin, *i.e.*,  $\mathbf{r} \rightarrow -\mathbf{r}, t \rightarrow -t$ .

Pauli first proposed and explained the strong reflection in [33] as follows: When the space-time coordinates change their sign, every particle transforms into its antiparticle simultaneously. The physical sense of the strong reflection is the substitution of every emission (absorption) operator of a particle by the corresponding absorption (emission) operator of its antiparticle. And there is no need to reverse the sign of the electric charge when the sign of space-time coordinates is reversed.

After combining with other necessary postulates, Lüders and Pauli proved that the Hamiltonian density of QFT (constructed from fields of spin zero, one-half and one by local interactions which are invariant under the proper Lorentz group) is invariant with respect to the strong reflection, which in turn is identical with the product of  $T$ ,  $C$  and  $P$  operations, thus completing the proof of CPT theorem [32].

The great merits of theoretical and experimental physicists working on P, C, CP and CPT problems should be highly appreciated because they gradually unveiled the essence of CPT theorem. What we are doing in this paper is merely to claim explicitly that the new postulate we have been seeking after for decades within our physics community is just the

CPT invariance itself, but in a simplified and better expression as shown by Eq.(31) because the postulate is emphasized from its beginning, *i.e.*, at the level of QM.

Actually, Eq.(31),  $\mathcal{PT} = \mathcal{C}$ , is just an explicit, also evolved form of the "strong reflection" invariance invented in the proof of CPT theorem. Following Pauli's idea, we emphasize that a particle's intrinsic property (especially, the distinction between a particle and its antiparticle) cannot be detached from the space-time. Hence we introduce the new notation  $\mathcal{PT}$  ( $\mathbf{x} \rightarrow -\mathbf{x}, t \rightarrow -t$ ) to represent the "strong reflection" explicitly and  $\mathcal{C}$  to stress that the correct particle-antiparticle transformation cannot be defined independently (like the old operator  $C$ ) but a direct consequence of the operation  $\mathcal{PT}$ . In other words, Eq.(31) is essentially a postulate injected implicitly into the theory from scratch (since the establishment of the theory of special relativity by Einstein in 1905), rather than a consequence of the CPT theorem.

Our readers may ask: "Besides discussions in previous sections, can Eq.(31) being something else which might be interesting?" We do think so. In the Appendix, the Klein paradox for both KG equation and Dirac equation is discussed at the level of QM in a consistent manner without resorting to the hole theory. Moreover, the invariance of a theory under the (newly defined) space-time inversion ( $\mathbf{r} \rightarrow -\mathbf{r}, t \rightarrow -t$ ) or the mass inversion ( $m \rightarrow -m$ ) in one coordinate frame could be used as a tool to find new equations which respect the symmetry between particle and its antiparticle (see [11, 13, 35]).

## Appendix: Klein Paradox for Klein-Gordon Equation and Dirac Equation

We will discuss the Klein paradox for both KG equation and Dirac equation based on the basic postulate, Eq.(31), at the level of QM.

### AI: Klein Paradox for KG Equation

Consider that a KG particle moves along  $z$  axis in one-dimensional space and hits a step potential

$$V(z) = \begin{cases} 0, & z < 0; \\ V_0, & z > 0. \end{cases} \quad (A.1)$$

Its incident WF with momentum  $p (> 0)$  and energy  $E (> 0)$  reads

$$\psi_i = a \exp[i(pz - Et)], \quad (z < 0) \quad (A.2)$$

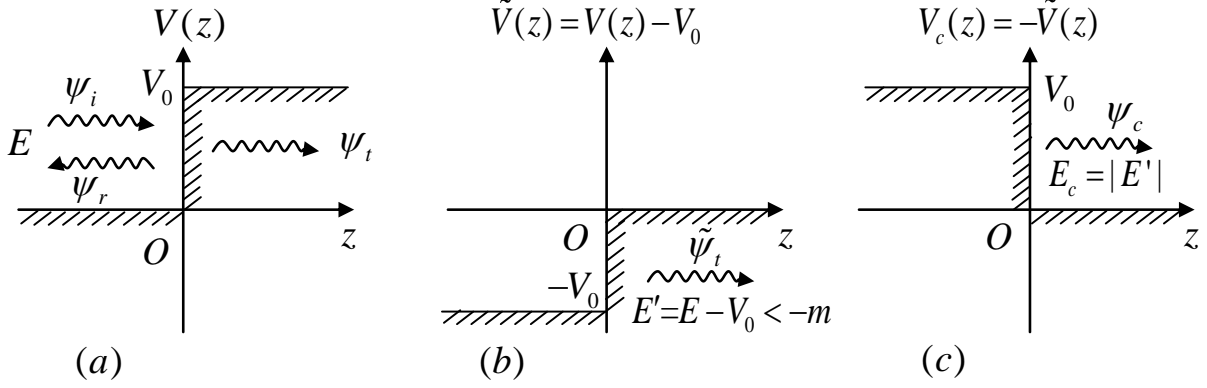


FIG. 1: Klein paradox: (a) If  $V_0 > E + m$ , there will be a wave  $\psi_t$  at  $z > 0$ .

(b) Just look at  $z > 0$  region, making a shift  $V(z) \rightarrow \tilde{V}(z) = V(z) - V_0$ ,  $E \rightarrow E' = E - V_0 < -m$ .

(c) An antiparticle (at  $z > 0$ ) appears with its energy  $E_c = |E'| > m$  and the potential is  $V_c(z) = -\tilde{V}(z)$

If  $E = \sqrt{p^2 + m^2} < V_0$ , we expect that the particle wave will be partly reflected at  $z = 0$  with WF  $\psi_r$  and another transmitted wave  $\psi_t$  emerged at  $z > 0$ :

$$\psi_r = b \exp[i(-pz - Et)], \quad (z < 0) \quad (\text{A.3})$$

$$\psi_t = b' \exp[i(p'z - Et)], \quad (z > 0) \quad (\text{A.4})$$

with  $p'^2 = (E - V_0)^2 - m^2$ . See Fig.1(a).

Two continuity conditions for WFs and their space derivatives at the boundary  $z = 0$  give two simple equations

$$\begin{cases} a + b = b' \\ (a - b)p = b'p' \end{cases} \quad (\text{A.5})$$

The Klein paradox happens when  $V_0 > E + m$  because the momentum  $p' = \pm \sqrt{(V_0 - E)^2 - m^2}$  is real again and the reflectivity  $R$  of incident wave reads

$$R = \left| \frac{b}{a} \right|^2 = \left| \frac{p - p'}{p + p'} \right|^2, \quad \begin{cases} R < 1, & \text{if } p' > 0 \\ R > 1, & \text{if } p' < 0 \end{cases} \quad (\text{A.6})$$

(See Ref.[6] or §9.4 in Ref.[11], where discussions were not complete and need to be complemented and corrected here). Because the kinetic energy  $E'$  at  $z > 0$  is negative:  $E' = E - V_0 < 0$ , what does it mean? Does the particle still remain as a particle?

As discussed in section IV, for a KG particle (or its antiparticle), two criterions must be held: its probability density  $\rho$  (or  $\rho_c$ ) must be positive and its probability current density  $\mathbf{j}$  (or  $\mathbf{j}_c$ ) must be in the same direction of its momentum  $\mathbf{p}$  (or  $\mathbf{p}_c$ ).

See Fig.1(b), after making a shift in the energy scale, *i.e.*, basing on the new vacuum at  $z > 0$  region, we redefine a WF  $\tilde{\psi}_t$  (which is actually the WF in the "interaction picture",  $\tilde{\psi}_t = \psi_t e^{iV_0 t}$  ( $z > 0$ ))

$$\psi_t \rightarrow \tilde{\psi}_t = b' \exp[i(p'z - E't)], \quad (z > 0) \quad (A.7)$$

( $E' = E - V_0 < 0$ ). From now on we will replace KG WF  $\tilde{\psi}_t$  by  $\tilde{\phi}_t$  and  $\tilde{\chi}_t$  according to Eq.(57), if  $\tilde{\psi}_t$  still describes a "particle", whose probability density  $\rho_t$  should be evaluated by Eq.(58) with  $V \rightarrow \tilde{V}(z) = 0$  ( $z > 0$ ) yielding:

$$\rho_t = |\tilde{\phi}_t|^2 - |\tilde{\chi}_t|^2 = \frac{E'}{m} |b'|^2 < 0, \quad (z > 0) \quad (A.8)$$

And its probability current density  $j_t$  should be given by Eq.(55), yielding:

$$j_t = \frac{p'}{m} |b'|^2, \quad (z > 0) \quad (A.9)$$

Eq.(A.8) is certainly not allowed. So to consider a "particle" with momentum  $p' > 0$  moving to the right makes no sense. Instead, we should consider  $p' < 0$  (which also makes no sense for a particle due to the boundary condition) and regard  $\tilde{\psi}_t$  as an antiparticle's WF by rewriting it as:

$$\tilde{\psi}_t = \psi_c = b' \exp[-i(p_c z - E_c t)], \quad (z > 0) \quad (A.10)$$

Now using Eq.(18) we see that Eq.(A.10) does describe an antiparticle with momentum  $p_c = -p' = |p'| = \sqrt{E_c^2 - m^2} > 0$  and energy  $E_c = |E'| = V_0 - E > 0$ . In the mean time, from the antiparticle's point of view (*i.e.*, with  $E_c > m$ ), the potential becomes  $V_c(z) = -\tilde{V}(z)$  (comparing Eq.(57) with Eq.(62)) as shown by Fig.1(c).

It is easy to see from Eqs.(61),(64) and (A.10) that[\*]

$$\begin{cases} \rho_t^c = |\tilde{\chi}_t^c|^2 - |\tilde{\phi}_t^c|^2 = \frac{E_c}{m} |b'|^2 > 0, \\ j_t^c = \frac{p_c}{m} |b'|^2 \end{cases} \quad (z > 0) \quad (A.11)$$

So the reflectivity, Eq.(A.6), should be fixed as:

$$R_{KG} = \left| \frac{b}{a} \right|^2 = \left| \frac{p + p_c}{p - p_c} \right|^2 = \left( \frac{1 + \gamma'}{1 - \gamma'} \right)^2, \quad \gamma' = \frac{p_c}{p} > 0 \quad (A.12)$$

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[\*] We had discarded the solution of  $p' > 0$  in Eqs.(A.8)-(A.9) as a particle. However, if we consider  $p' = -p_c > 0$  for an antiparticle, then similar to Eqs.(A.10)-(A.11), we would get  $\rho_t^c > 0$  but both  $j_t^c$  and  $p_c$  are negative, meaning that the antiparticle is coming from  $z = \infty$ , not in accordance with our boundary condition. So the case of  $p' > 0$  should be abandoned either as a particle or as an antiparticle.

And the transmission coefficient can also be predicted as:

$$T_{KG} = \frac{j_t^c}{j_i} = \frac{p_c}{p} \left| \frac{b'}{a} \right|^2 = \frac{p_c}{p} \left| 1 + \frac{b}{a} \right|^2 = \frac{4pp_c}{(p - p_c)^2} = \frac{4\gamma'}{(1 - \gamma')^2} \quad (A.13)$$

$$R_{KG} - T_{KG} = 1 \quad (A.14)$$

The variation of  $T_{KG}$  seems very interesting:

$$T_{KG} = \begin{cases} 0, \gamma' \rightarrow 0 & (p_c \rightarrow 0, E_c \rightarrow m) \\ \infty, \gamma' \rightarrow 1 & (p_c = p, E_c = E = V_0/2) \\ 0, \gamma' \rightarrow \infty & (p_c \rightarrow \infty, E_c = V_0 - E \rightarrow \infty) \\ 0, \gamma' \rightarrow \infty & (p \rightarrow 0, E \rightarrow m) \end{cases} \quad (A.15)$$

Above equations show us that the incident KG particle triggers a process of "pair creation" occurring at  $z = 0$ , creating new particles moving to the left side (to join the reflected incident particle) so enhancing the reflectivity  $R_{KG} > 1$  and new antiparticles (with equal number of new particles) moving to the right.

To our understanding, this is not a stationary state problem for a single particle, but a nonstationary creation process of many particle-antiparticle system. It is amazing to see the Klein paradox in KG equation being capable of giving some prediction for such kind of process at the level of RQM. Further investigations are needed both theoretically and experimentally. [†]

### AII: Klein Paradox for Dirac Equation

Beginning from Klein [27], many authors *e.g.* Greiner *et al.* [36, 37], have studied this topic. We will join them by using the similar approach like that for KG equation discussed above.

Based on similar picture shown in Fig.1, now we have three Dirac WFs under the condition  $V_0 > E + m$ :

$$\psi_i = a \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E+m} \\ 0 \end{pmatrix} e^{i(pz-Et)}, \psi_r = b \begin{pmatrix} 1 \\ 0 \\ \frac{-p}{E+m} \\ 0 \end{pmatrix} e^{i(-pz-Et)} \quad (z < 0) \quad (A.16)$$

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[†] We find from the Google search that R. G. Winter in 1958 had examined the Klein paradox for KG equation at the QM level and reached basically the same result as ours. So he was the first author dealing with this problem. Regrettably, it seems that his paper had never been published on some journal.

$$\psi_t = b' \begin{pmatrix} 1 \\ 0 \\ \frac{p'}{E-V_0+m} \\ 0 \end{pmatrix} e^{i(p'z-Et)} = b' \begin{pmatrix} 1 \\ 0 \\ \frac{-p'}{V_0-E-m} \\ 0 \end{pmatrix} e^{i(p'z-Et)} = \begin{pmatrix} \phi_t \\ \chi_t \end{pmatrix} \quad (z > 0) \quad (\text{A.17})$$

where  $p' = \pm \sqrt{(V_0 - E)^2 - m^2}$ . Unlike Eq.(A.8) for KG equation, the probability density for Dirac WF  $\psi_t$  is positive definite (see Eq.(84))

$$\rho_t = \psi_t^\dagger \psi_t = \phi_t^\dagger \phi_t + \chi_t^\dagger \chi_t \quad (\text{A.18})$$

Hence we will rely on two criterions: First, the probability current density and momentum must be in the same direction for either a particle or antiparticle. For  $\psi_i$  and  $\psi_r$ , their probability current density are ( $c = 1$ )

$$\begin{aligned} j_i &= \psi_i^\dagger \alpha_z \psi_i = \phi_i^\dagger \sigma_z \chi_i + \chi_i^\dagger \sigma_z \phi_i = \frac{2p}{E+m} |a|^2 > 0 \\ j_r &= \psi_r^\dagger \alpha_z \psi_r = \frac{-2p}{E+m} |b|^2 < 0 \end{aligned} \quad (z < 0) \quad (\text{A.19})$$

as expected. However, for  $\psi_t$ , we meet difficulty similar to that in Eq.(A.9)

$$j_t = \psi_t^\dagger \alpha_z \psi_t = \frac{-2p'}{V_0 - E - m} |b'|^2 \quad (z > 0) \quad (\text{A.20})$$

the direction of  $j_t$  is always opposite to that of  $p'$ ! The second criterion is: while  $|\phi| > |\chi|$  for particle, we must have  $|\chi_c| > |\phi_c|$  for antiparticle. Now in  $\psi_i$  (or  $\psi_r$ ),  $|\phi_i| > |\chi_i|$  (or  $|\phi_r| > |\chi_r|$ ), but the situation in  $\psi_t$  is dramatically changed, the existence of  $V_0$  renders  $|\chi_t| > |\phi_t|$ !

The above two criterions, together with the experience in KG equation, prompt us to choose  $p' < 0$  and regard  $\psi_t$  as an antiparticle's WF. So we rewrite:

$$\psi_t = \psi_t^c e^{-iV_0 t} \quad (\text{A.21a})$$

$$\psi_t^c = b' \begin{pmatrix} 1 \\ 0 \\ \frac{p_c}{E_c-m} \\ 0 \end{pmatrix} e^{-i(p_c z - E_c t)} = \begin{pmatrix} \phi_t^c \\ \chi_t^c \end{pmatrix}, \tilde{\psi}_t^c = b'_c \begin{pmatrix} 1 \\ 0 \\ \frac{p_c}{E_c+m} \\ 0 \end{pmatrix} e^{-i(p_c z - E_c t)} = \begin{pmatrix} \chi_t^c \\ \phi_t^c \end{pmatrix} \quad (z < 0) \quad (\text{A.21b})$$

where  $\tilde{\psi}_t^c = (-\gamma^5) \psi_t^c$  (with new normalization constant  $b'_c$  replacing  $b'$ ) describes an antiparticle with momentum  $p_c = |p'| = -p' = \sqrt{E_c^2 - m^2} > 0$ , energy  $E_c = V_0 - E > 0$  and  $|\chi_t^c| > |\phi_t^c|$ . Using Eq.(85) we find

$$j_t^c = \frac{2p_c}{E_c + m} |b'_c|^2 > 0, \quad (z > 0) \quad (\text{A.22})$$

as expected. Now it is easy to match Dirac WFs at the boundary  $z = 0$ ,  $(\psi_i + \psi_r)|_{z=0} = \tilde{\psi}_t^c|_{z=0}$ , yielding[\*]

$$\begin{cases} a + b = b'_c \\ \frac{(a - b)p}{E + m} = \frac{b'_c p_c}{E_c + m} \end{cases} \rightarrow \begin{cases} \frac{b}{a} = \frac{\xi - \eta}{\xi + \eta} \\ \frac{b'_c}{a} = 1 + \frac{b}{a} = \frac{2\xi}{\xi + \eta} \end{cases} \quad (\text{A.23})$$

where  $\xi = p(E_c + m) > 0, \eta = p_c(E + m) > 0$ . The reflectivity  $R_D$  and transmission coefficient  $T_D$  follow from Eq.(A.19) and (A.22) as:

$$R_D = \frac{|j_r|}{j_i} = \left| \frac{b}{a} \right|^2 = \left( \frac{1 - \gamma}{1 + \gamma} \right)^2 \quad (\text{A.24})$$

$$T_D = \frac{j_t^c}{j_i} = \left| \frac{b'_c}{a} \right|^2 \frac{p_c(E + m)}{p(E_c + m)} = \frac{4\gamma}{(1 + \gamma)^2} \quad (\text{A.25})$$

$$R_D + T_D = 1 \quad (\text{A.26})$$

where

$$\gamma = \frac{\eta}{\xi} = \sqrt{\frac{(E_c - m)(E + m)}{(E - m)(E_c + m)}} \geq 0 \quad (E_c = V_0 - E \geq m) \quad (\text{A.27})$$

and

$$T_D = \begin{cases} 0, \gamma \rightarrow 0 & (p_c \rightarrow 0, E_c \rightarrow m) \\ 1, \gamma = 1 & (p_c = p, E_c = E = V_0/2) \text{ (resonant transmission)} \\ \frac{2p}{E+p}, \gamma \rightarrow \sqrt{\frac{E+m}{E-m}} & (E_c = V_0 - E \rightarrow \infty) \\ 0, \gamma \rightarrow \infty & (p \rightarrow 0, E \rightarrow m) \end{cases} \quad (\text{A.28})$$

The variation of  $T_D$  bears some resemblance to Eq.(A.15) for KG equation but shows striking difference due to sharp contrast between Eqs.(A.24)-(A.28) and Eqs.(A.12)-(A.15).

To our understanding, in the above Klein paradox for Dirac equation, there is no "pair creation" process occurring at the boundary  $z = 0$ . The paradox just amounts to a steady transmission of particle's wave  $\psi_i$  into a high potential barrier  $V_0 > E + m$  at  $z > 0$  region where  $\psi_t$  shows up as an antiparticle's WF propagating to the right. In some sense, the existence of a potential barrier  $V_0$  plays a "magic" role of transforming the particle into its

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[\*] Eq.(A.23) means that the large (small) component of spinor is connected with large (small) component at both sides of  $z = 0$ . However, if instead of  $\tilde{\psi}_t^c$ , the  $\psi_t^c$  is used directly with its first (small) component being connected with the first (large) components of  $\psi_i$  and  $\psi_r$ , it would lead to a different expression of Eq.(A.27):  $\gamma \rightarrow \tilde{\gamma} = \sqrt{\frac{(E_c - m)(E - m)}{(E + m)(E_c + m)}}$ , which is just the  $1/\gamma$  ( $\gamma$  and  $1/\gamma$  make no difference in the result of, say, Eqs.(A.24) and (A.25)) defined by Eq.(8) on page 266 of Ref.[36] (see Eq.(A31) below) or that by Eq.(5.36) in Ref.[37]

antiparticle. Because the probability densities of both particle and antiparticle are positive definite, the total probability can be normalized over the entire space like that for one particle case:

$$\int_{-\infty}^{\infty} [\rho(z)\Theta(-z) + \rho_c(z)\Theta(z)]dz = 1 \quad (\text{A.29})$$

( $\Theta(z)$  is the Heaviside function) and the probability current density remains continuous at the boundary  $z = 0$ . In other words, the continuity equation holds in the whole space just like what happens in a one-particle stationary state.

It is interesting to compare our result with that in Refs.[36] and [37]. In Ref.[36], Eqs.(13.24)-(13.28) are essentially the same as ours. But the argument there for choosing  $\bar{p} < 0$  in Eq.(13.23) is based on the criterion of the group velocity  $v_{gr}$  being positive (for the transmitted wave packet moving toward  $z = \infty$ ). And the  $v_{gr}$  is stemming from Eq.(13.16) which is essentially the probability current density in our Eq.(A.19) or (A.20).

However, the author in Ref.[36] also considered the other choice  $\bar{p} > 0$  in the example (p.265-267 in [36]) based on the hole theory, ending up with the prediction as:

$$R = \left( \frac{1 + \gamma}{1 - \gamma} \right)^2, \quad T = \frac{4\gamma}{(1 - \gamma)^2}, \quad R - T = 1 \quad (\text{A.30})$$

where

$$\gamma = \frac{p_2}{p_1} \frac{E + m}{V_0 - E - m} = \sqrt{\frac{(V_0 - E + m)(E + m)}{(V_0 - E - m)(E - m)}} \quad (\text{A.31})$$

The argument for the validity of his Eqs.(A.30)-(A.31) is based on the hole theory (see also section 5.2 in Ref.[37]), saying that once  $V_0 > E + m$ , there would be an overlap between the occupied negative continuum for  $z > 0$  and the empty positive continuum for  $z < 0$ , providing a mechanism for electron-positron pair creation if the "hole" at  $z > 0$  can be identified with a positron. We doubt the "hole" theory seriously because there are only two electrons (with opposite spin orientations) staying at each energy level in the negative continuum. So it seems that there is no abundant source for electrons and "holes" to account for the huge value of  $T > 1$  in Eq.(A.30).

Fortunately, we learn from section 10.7 in Ref.[37] that if the Klein paradox in Dirac equation is treated at the level of QFT, their result turns out to be the same form as our Eqs.(A.24)-(A.28), rather than Eqs.(A.30)-(A.31).



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